

Discovery of deuterated water in a young proto-planetary disk

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ABSTRACT

We report the first detection of the ground transition of the deuterated water at 464 GHz in the young proto-planetary disk surrounding the solar type protostar DM Tau. The line is observed in absorption against the continuum from the cold dust in the disk midplane, with a line to continuum ratio close to unity. The observation implies that deuterated gaseous water is present, with a relatively large abundance ($\sim 3 \times 10^{-9}$), in the outer disk above the midplane, where the density is, within a factor ten, $\sim 10^6 \text{ cm}^{-3}$ and the temperature is lower than about 25 K. In these conditions, the H_2O condensation timescale is much smaller than the DM Tau disk age, and, therefore, water should be fully frozen onto the grain mantles. We suggest that UV photons and/or X-rays sublimate part of the mantles re-injecting the ices into the gas phase. Even though there is currently no measurement of H_2O , we provide arguments that the $\text{HDO}/\text{H}_2\text{O}$ ratio should be about 0.01 or larger, which would be hundreds of times larger than the values measured in Solar System objects. This suggests the need of strong caution in comparing and linking the $\text{HDO}/\text{H}_2\text{O}$ in Solar System and star forming environments.

Subject headings: Stars: formation – Stars: protoplanetary disks – Stars: Pre-main-sequence – ISM: molecules –

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1. Introduction

Water is an important molecule to study during the formation of solar type stars for several reasons. It is one of the most abundant molecules in the material surrounding a forming star, and it is the most abundant molecule after H_2 and CO in the innermost regions of the low mass protostellar envelopes (Ceccarelli et al. 2000). Since water has a very large dipole moment, it is a very efficient coolant of the gas, and can therefore dominate its thermal balance (Ceccarelli et al. 1996). Finally, because it can be a major reservoir of the oxygen element, water also regulates the chemistry of other less abundant oxygen-bearing molecules (Roberts & Herbst 2002).

Deuterated water in solar type forming stars is also important because of the link with the comets and the Earth oceans. Until recently, it was thought that the terrestrial water came from the outer (≥ 2.5 AU) Solar System, brought by colliding bodies after the Earth formation (Owen & Bar-Nun 1995). This theory is now challenged by a new class of dynamical simulations which theorize on the simultaneous formation of the oceans and the Earth (Raymond et al. 2004; Gomes et al. 2005), but these ideas are still much debated. A key indicator in the puzzle about the ocean formation is provided by the so-called Standard Mean Ocean Water (SMOW) $\text{HDO}/\text{H}_2\text{O}$ ratio (Table 3). This value is about ten times larger than the elemental Deuterium/Hydrogen ratio in the Solar nebula, and similar to the values measured in comets and carbonaceous chondrites (Table 3). The origin of the $\text{HDO}/\text{H}_2\text{O}$ ratio in both comets and meteorites is also very debated (Bockelee-Morvan et al. 1998). It is often compared to what is observed in the Interstellar Medium (ISM), either in the cold clouds from where stars form or in the hot cores of *massive* protostars, which possess $\text{HDO}/\text{H}_2\text{O}$ values close to the SMOW (Meier et al. 1998). However, recent observations in protostars with *masses similar to the Sun* measure a $\text{HDO}/\text{H}_2\text{O}$ value larger than the SMOW by about two orders of magnitude (Parise et al. 2005, see below), so that the match is likely a coincidence. Therefore, the question about the origin of the $\text{HDO}/\text{H}_2\text{O}$ ratio in comets, asteroids and the oceans is still open. In particular, it is not clear whether the $\text{HDO}/\text{H}_2\text{O}$ is preserved during the last phase before the formation of the planetary system, the phase of the proto-planetary disk. And no direct observations exists so far of the water content and/or the $\text{HDO}/\text{H}_2\text{O}$ ratio in systems similar to the progenitor of the Solar System.

Molecular deuteration in the ISM and in star forming regions has recently been the target of a flurry of activity, initiated by the discovery of multiply deuterated molecules in solar-type protostars (e.g. see the review by Ceccarelli 2002), where D/H ratios are enhanced by up to 13 orders of magnitude with respect to the elemental D/H ratio (Parise et al. 2004). This extreme enrichment occurs during the initial stages of cloud collapse in the Pre-Stellar-Phase (Bacmann et al. 2003). Low temperatures and high densities lead to freeze-out of the

molecules onto the grain mantles, and to enhanced deuteration of H_3^+ , the most abundant molecular ion in such a gas, which “transmits” the deuteration to the other molecules (Caselli et al. 2003). In the subsequent protostar phase, heating of the dust leads to the sublimation of ices in the inner ~ 100 AU, injecting ice molecules back into the gas phase (Ceccarelli et al. 2000).

Water, however, seems to follow a different path. While the abundance of singly deuterated isotopomers of H_2CO and CH_3OH are more than 1/3 of the the main isotopomers, HDO is less than 3% of H_2O in solar-type protostars (Parise et al. 2005). Specifically, $\text{HDO}/\text{H}_2\text{O}$ is equal to 0.03 in the region where water ices sublimate, and less than 0.002 in the outer envelope, where the water abundance is dominated by gas-phase reactions. The reason for this different behavior most likely lies in the formation process. Since water has a large dipole, it freezes out onto the grain mantles already at ~ 90 K (Fraser et al. 2001). Therefore the reactions forming water and water ice can occur at relatively high temperatures, when the H_3^+ deuteration is limited. On the other hand, formaldehyde and methanol are believed to be formed by hydrogenation of frozen CO (Tielens & Hagen 1982). Since the condensation temperature of CO is ~ 25 K (Öberg et al. 2005), this forces these reactions to take place at very low temperatures. Under those conditions, the enhanced D/H of the accreting atomic gas leads to high deuterium fractionation of molecules formed by CO hydrogenation on grains (e.g. Tielens & Hagen 1982).

After the dispersion of the protostar envelope, a proto-planetary disk is left over from which asteroids, comets and planets may form. The key questions to answer to improve our understanding of the origin of the terrestrial water are: is there enough H_2O and HDO in a proto-planetary disk (similar to what could have been the Solar Nebula) to account for the water and ice present in the solar system? What is the $\text{HDO}/\text{H}_2\text{O}$ ratio across the disk? Is the $\text{HDO}/\text{H}_2\text{O}$ of the pre-collapse and embedded protostar phases preserved during the proto-planetary disk phase? And, ultimately, what is the origin of deuteration in comets, meteorites and oceans?

In this Letter we report the discovery of deuterated water in the disk surrounding DM Tau, a T Tauri star at 140 pc from the Sun. An extended disk of molecular gas has been first discovered by Guilloteau & Dutrey (1994). Subsequently Dutrey et al. (1997) carried out a survey of different molecules. The dust disk mass is $2 \times 10^{-4} M_\odot$, and the age is estimated to be around 5 Myr. Finally, the disk has a diameter of $12''$ ($= 800$ AU in radius).

2. Observations and results

The ground ($1_{0,1}-0_{0,0}$) transition of HDO at $\nu = 464.92452$ GHz was observed on February 20, 22 and 28, 2005 with the JCMT near the summit of Mauna Kea in Hawaii, USA. The observations were performed with the dual-polarization W(C) receiver in single-sideband mode. At the time of the observations, only one polarization was active. It was connected to a unit of an autocorrelator providing a bandwidth of 250 MHz for a spectral resolution of 156 kHz for some scans, and a bandwidth of 500 MHz for a spectral resolution of 312 kHz for others. All data were smoothed to the lowest spectral resolution, yielding a velocity resolution of about 0.2 km s^{-1} . The observations were performed in beam switching mode with a throw of $180''$. Pointing and focus were regularly checked using planets or strong sources, providing a pointing accuracy of about $3''$. The telescope beam at 464 GHz is $11''$, and the main beam efficiency is 0.45 (as reported on the JCMT Manual: http://www.jach.hawaii.edu/JCMT/spectral_line/).

The data have been reduced with the GILDAS package CLASS. The total integration time spent on the source was about 7.2 hours with a zenith τ opacity at 225 GHz better than 0.06. Nevertheless, some scans were taken at a high zenith angle, yielding to drift in calibration, and higher noise. We therefore dropped the scans with observed $\tau \geq 0.23$ to build the final used dataset. The integration time of this final dataset is 5.5 hours, and the main beam temperature rms is equal to 33 mK in a 0.2 km s^{-1} bin.

Figure 1 shows the spectrum observed towards DM Tau. Two absorption features are detected with a Signal-to-Noise (S/N) ratio better than 3: the first one coincides exactly with the ground transition of HDO (at 464.9245 GHz) when the systemic velocity (5.5 km s^{-1}) of DM Tau is taken into account. The other absorption feature at 11 km s^{-1} is due to a C_6H transition at 464.9172 GHz¹. In order to check the robustness of the detection, we analyzed all the obtained data in multiple subsets of data, and the absorptions feature are present in all of them, regardless of the definition of the datasets. This test ensures that the features are indeed the result of summing all the spectra and not due to a strong fluctuation in a few ones. All together, this gives substantial support to the reality of the HDO absorption. We postpone the discussion about the C_6H detection to a forthcoming article (Dominik et al. in preparation). Here we focus on the HDO detection, the first ever in a proto-planetary disk. The velocity-integrated HDO line is $(-0.075 \pm 0.019) \text{ K km s}^{-1}$ (main beam temperature), and the linewidth is $(0.63 \pm 0.18) \text{ km s}^{-1}$.

¹The C_6H identification is firmly established thanks to the presence of another absorption feature at 465.0511 GHz from the same molecule in the spectrum, and to the detection of the same two C_6H lines towards another disk source, during the same observation run (Dominik et al. in preparation).

A continuum at 464 GHz of 2 Jy, derived by modeling of the Spectral Energy Distribution (SED: see Figure 2 and the text below), gives a line to continuum ratio of 0.9 (i.e. the relative depth of the absorption line is close to 1). This corresponds to an absorbing HDO column density equal to $8 \times 10^{12} \text{ cm}^{-2}$. This number is based on the assumption that all HDO molecules are in the ground state, which is a valid assumption for the involved gas temperature and density. The uncertainty associated with the derived line to continuum ratio and HDO column density is around a factor 2, when considering the uncertainty in the modeling and the observed line absorption (close to unity). However, the line may be optically thick and, in which case the derived column density would be a lower limit to the real HDO column density.

3. Discussion

In order to correctly interpret the meaning of the HDO line, the first question to answer is: what is the location of the HDO molecules causing the absorption? Is it gas in the (cold) upper layers of the outer disk ($r \geq 30 \text{ AU}$), or gas in the (warm) midplane close to the star? The answer to this question is straightforward. The photons which are absorbed by the HDO molecules in the line of sight are emitted by cold dust ($\sim 10 \text{ K}$), therefore by dust in the outer midplane. As a consequence, *the HDO molecules must be in the gas above the outer midplane*. Furthermore, because the line-to-continuum ratio is close to unity, *the HDO gas must cover most of the disk*. Finally, the fact that the line is in absorption and not in emission implies that the gas with HDO has a relatively low density, below the critical density of the transition. The latter is $\sim 3 \times 10^9 \text{ cm}^{-3}$ at 20 K (Grosjean et al. 2003). *We conclude that HDO (and therefore H_2O) vapor is present in the outer disk above the midplane, at a density less than $\sim 10^8 \text{ cm}^{-3}$* . Since only the gas towards us absorbs the 464 GHz photons, the total HDO molecules are twice the HDO column density required to absorb the continuum, namely $N(\text{HDO}) \sim 1.6 \times 10^{13} \text{ cm}^{-2}$, to account for the other side of the disk. This implies a gaseous HDO mass in the disk equal to $\sim 2 \times 10^{23} \text{ gr}$, which is about 850 times the amount of HDO in the terrestrial oceans. Again, if the line is optically thick, all numbers are lower limits.

Figure 3 shows the physical structure of DM Tau, derived by modeling the SED (Fig. 2). For that we used a passive disk model with an inner hole (Dullemond et al. 2001), computed with 1+1D treatment of radiative transfer and self-consistent vertical structure (Dullemond et al. 2002). In “standard” conditions, H_2O molecules condense out onto the grain mantles at a rate:

$$k_{\text{dep}} = S \pi a_{\text{gr}}^2 n_{\text{g}} \langle v_{\text{H}_2\text{O}} \rangle \quad (1)$$

and are released back into the gas phase by thermal evaporation, at a rate (Hasegawa & Herbst 1993):

$$k_{\text{ev}} = \nu_0 \exp[-E_{\text{b}}/kT] \quad (2)$$

In Eq. (1), S is the sticking coefficient, a_{gr} is the mean grain radius ($0.1 \mu\text{m}$), n_{g} is the grain number density (with respect to H_2 , equal to 3.2×10^{-12}), and $v_{\text{H}_2\text{O}}$ is the H_2O thermal velocity. In Eq. (2), $\nu_0 = 10^{12}\text{s}^{-1}$ is the frequency of oscillation between adsorbate and surface and E_{b} is the binding energy per molecule. Note that, in contrast to CO , cosmic rays do not contribute significantly to the release of H_2O from the ice (Hasegawa & Herbst 1993). Taking the standard value for the sticking coefficient (larger than 0.3), and the H_2O binding energy measured by laboratory experiments ($\sim 5600 \text{ K}$; Fraser et al. 2001) leads to all the water frozen onto the grain mantles at a distance larger of $\sim 30 \text{ AU}$ in much less than the estimated age of DM Tau ($\sim 5 \text{ Myr}$). This is a well known effect in the literature of the Solar Nebula studies, giving rise to the “snow-line” (Davis 2005). Therefore no vapor water should be present in the outer disk. However, *we do observe HDO in the gas phase, in significant quantities and this is the first important conclusion of the present work.*

In order to compute the HDO abundance, we need to estimate the H_2 column density in the region where the absorbing HDO is located. Using the physical structure derived from the SED modeling (Fig. 3), the H_2 column density of the gas at 600-800 AU is about $3 \times 10^{21} \text{ cm}^{-2}$, if the gas is located at a height of about 300 AU (corresponding to a density of $\sim 10^6 \text{ cm}^{-3}$). If the HDO absorption is located closer to the midplane, at densities $\sim 10^7 \text{ cm}^{-3}$, the H_2 column density would be a factor three larger. In the unlikely case (see below) that the absorption originates higher in the disk, the H_2 column density could be a factor three lower. This implies a HDO abundance (with respect to H_2) of $\sim 3 \times 10^{-9}$, with an uncertainty of about a factor three, depending how deep in the disk the HDO gas lies. Unfortunately, observations of H_2O are impossible from the ground, and we need to wait for the advent of the Herschel Space Observatory for an actual measure of the H_2O abundance in the gas phase². However, we can compare the derived HDO abundance with the observations of H_2O in molecular clouds and protostars, $\sim 3 \times 10^{-7}$ (Cernicharo et al. 1997; Bergin et al. 2003; Maret et al. 2002), and this would give $\text{HDO}/\text{H}_2\text{O}$ equal to ~ 0.01 . If, on the other hand, the water abundance is lower and more similar to what is measured in cold molecular clouds, $\leq 10^{-8}$ (Bergin & Snell 2002), the $\text{HDO}/\text{H}_2\text{O}$ ratio would be larger than 0.3. Therefore, the second conclusion of the present work is that *the vapor HDO/ H_2O ratio in the proto-planetary disk surrounding DM Tau is probably larger than 0.01, unless the abundance of the water is larger than $\sim 3 \times 10^{-7}$.*

²Neither SWAS nor ODIN have the sensitivity enough for the detection of water in DM Tau, unless the H_2O abundance is much larger than 3×10^{-7} .

In summary, the HDO detection proves that water vapor is present in the outer disk, in the layers above the midplane where the temperature is lower than about 25 K and density is, within a factor ten, $\sim 10^6 \text{ cm}^{-3}$, and that the HDO/H₂O ratio is likely larger than 0.01. We explore now what this implies. First, the timescale for condensation of water molecules at 10^6 cm^{-3} is $\sim 10^4 \text{ yr}$ (Eq. 1), whereas the estimated age of the disk is of a few million years. Therefore, the condensation of water molecules onto grains is either slowed down significantly, or countered by continuously “sublimation” of the icy grain mantles. We are not aware of any physical process capable of slowing down condensation of water onto the grain mantles. We therefore consider the possible mechanisms that would make the icy grain mantles sublimate. The first possibility is that UV photons photo-desorb the icy mantles. Where UV photons penetrate, they also photo-dissociate the water molecules, keeping the steady-state abundance of water molecules low and limited to a narrow region. It is unclear whether the resulting column density is enough to explain the observations. Shocks from possible turbulent mixing from the low to the upper layers (vertical mixing) would be too slow ($\leq 1 \text{ km s}^{-1}$) and weak to give any appreciable effect. The same applies to any accretion shock in the outer disk. Another possibility is that X-rays spot-heat the grain mantles making part of them sublimate (Najita et al. 2001). Indeed, T Tau stars are known to be strong X-rays emitters (Feigelson & Montmerle 1999), and a preliminary analysis of CHANDRA observations suggests X-rays emission associated with DM Tau (M. Guedel, private communication). Thus, X-rays would be, in this sense, a natural explanation (see also Bergin et al. (2004)), although it is difficult to quantify the amount of sublimated ice.

Finally, Table 1 lists the measurements of the HDO/H₂O ratio in objects representing different stages of the formation of a solar type star, compared to the measurements in the Solar System. Although the HDO/H₂O ratio in comets and carbon chondrites is 10 times larger than the elemental D/H ratio, it is much smaller than the value observed during the protostellar phase of a solar type star, and, likely, also smaller than the value measured during the final phase, namely the proto-planetary disk phase. However, our observations strictly refer to the outer disk, at a scale much larger than where comets and carbon meteorites are thought to originate. Therefore, it will be paramount to have the *spatial distribution* of the HDO/H₂O ratio across the proto-planetary disks. Our observations show that these studies can be done searching for the *absorption* of the ground state of HDO and, likely, H₂O lines. The future interferometric instrument ALMA will represent a unique opportunity for these studies. As a final remark, the present study confirms that caution is mandatory in linking the HDO/H₂O ratio in Solar System objects to star forming environments.

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Source	HDO/H ₂ O	Reference
Solar Nebula	1.5×10^{-5}	1
Earth Oceans	1.6×10^{-4}	2
Carbonaceous Chondrites	$\sim 1.5 \times 10^{-4}$	3
Comets	$\sim 3 \times 10^{-4}$	4
Proto-Planetary Disk	~ 0.01	5
Class 0 Protostar Sublimated Ices	~ 0.03	6

Table 1: The HDO/H₂O ratio in sources representing different stages of the formation of a solar type star, together with the values measured in the Solar System. References: 1- Geiss (1993); 2- De Witt et al. (1980); 3- Robert et al. (2000); 4- Meier et al. (1998) ;5- present work; 6- Parise et al. (2005).

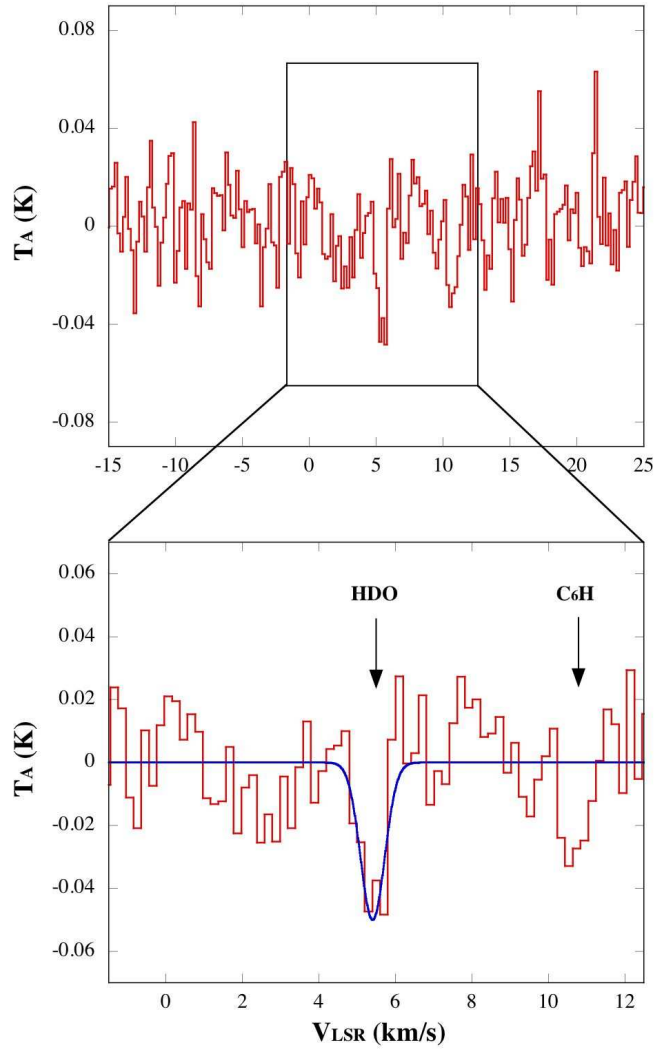


Fig. 1.— The observed line spectrum of DM Tau at 464 GHz. The HDO ground transition, and the C₆H transition are marked by lines.

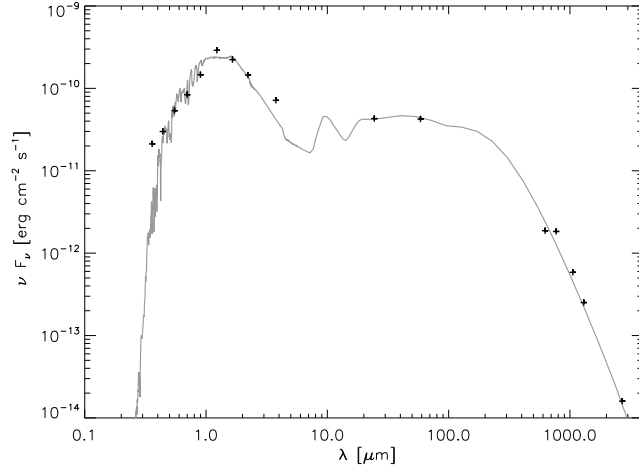


Fig. 2.— The observed Spectral Energy Distribution in DM Tau. Crosses represent observations, while the solid line shows the modeled SED, using the model described in the text. The disk has a mass of $0.023 M_{\odot}$, a surface density distribution $\propto r^{-1.5}$, in a disk reaching out to 800 AU from the star. We used a stellar mass of $0.65 M_{\odot}$, effective temperature of 3630 K and a luminosity of $0.28 L_{\odot}$. For fitting the observations, a distance of 140 pc has been assumed. The structure resulting from this model is shown in Fig. 3.

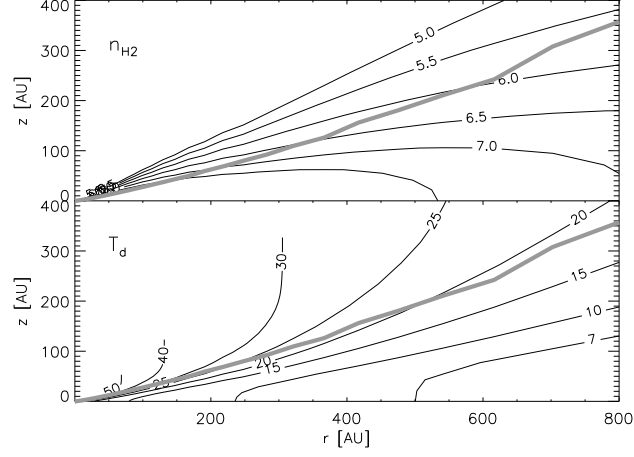


Fig. 3.— The logarithm of the density (upper panel) and the temperature (lower panel) of the disk surrounding DM Tau, as derived by modeling of the SED (Fig. 2). The thick line shows the disk surface, i.e. the location where the disk reaches an optical depth of unity for grazing stellar photons.